

Relativistic particle in a three-dimensional box

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We generalize the work of Alberto, Fiolhais and Gil and solve the problem of a Dirac particle confined in a 3-dimensional box. The non-relativistic and ultra-relativistic limits are considered and it is shown that the size of the box determines how relativistic the low-lying states are. The consequences for the density of states of a relativistic fermion gas are briefly discussed.

I. INTRODUCTION

The problem of a particle confined in an one-dimensional infinite square well potential lies at the heart of non-relativistic quantum mechanics, being the simplest problem that illustrates how the wave nature of bound particles implies that their energy is quantized. The generalization of this problem to three dimensions is used for the statistical description of a fermion gas and is the starting point for some many-body theories of fermions like the Thomas-Fermi model of the atom.

The relativistic formulation and solution of the problem of a spin-1/2 fermion with mass m confined in a one-dimensional square well potential was done by Alberto, Fiolhais and Gil [1]. In this paper we review their approach and generalize it to a 3-dimensional square well potential. The problem of a relativistic particle confined in infinite square well potential is traditionally not dealt with in the textbooks of Relativistic Quantum Mechanics, even in the most comprehensive ones such as the one by Greiner [2].

Recently, in the context of quantum gravity phenomenology, applications of this result were presented. In particular, by applying the Generalized Uncertainty Principle (GUP) to a particle confined in a three-dimensional box, it is shown that the length of the box must be quantized in terms of a fundamental length, e.g. Planck length, and this indicates that the nature of space may be fundamentally grainy [3].

In the present analysis, we choose an ansatz for the spinor inside the box which is consistent with the non-relativistic problem and derive a transcendental equation for the wave numbers allowed. We obtain the non-relativistic and ultra-relativistic limits of this equation and its solutions, showing also how they are related to the ratio between the size of the containing box and the Compton wavelength $\hbar/(mc)$ of the fermion. Finally, we discuss briefly the differences regarding the density of states between the usual non-relativistic fermion gas and the relativistic fermion gas.

II. SOLUTION OF DIRAC EQUATION WITH A ONE DIMENSIONAL INFINITE SQUARE WELL

The Dirac equation is written as ¹

$$\begin{aligned} H\psi &= (c\vec{\alpha} \cdot \vec{p} + \beta mc^2) \psi(\vec{r}) \\ &= E\psi(\vec{r}) \end{aligned} \tag{1}$$

where α_i ($i = 1, 2, 3$) and β are the Dirac matrices, for which we use the following representation

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{2}$$

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¹ In this section, we follow the formulation of [1].

where σ_i are the Pauli matrices and I is the 2-dimensional unit matrix. It is evident that in 1-spatial dimension and in the position representation, say z , the Dirac equation is given by

$$\left(-i\hbar c\alpha_z \frac{d}{dz} + \beta mc^2\right) \psi(z) = E\psi(z) . \quad (3)$$

The positive energy solutions read

$$\psi = N e^{ikz} \begin{pmatrix} \chi \\ r\sigma_z\chi \end{pmatrix}$$

where m is the mass of the Dirac particle, k is the wavenumber that satisfies the usual dispersion relation $E^2 = (\hbar kc)^2 + (mc^2)^2$, $r \equiv \frac{\hbar kc}{E+mc^2}$ and $\chi^\dagger\chi = 1$. Note that r runs from 0 (non-relativistic) to 1 (ultra-relativistic), k could be positive (right moving) or negative (left moving), while N is a suitable normalization constant.

As noted in [1], to confine a relativistic particle in a box of length L in a consistent way avoiding the Klein paradox (in which an increasing number of negative energy particles are excited), one may take its mass to be z -dependent as was done in the MIT bag model of quark confinement [4, 5]

$$m(z) = M, \quad z < 0 \quad (\text{Region I}) \quad (4)$$

$$= m, \quad 0 \leq z \leq L \quad (\text{Region II}) \quad (5)$$

$$= M, \quad z > L \quad (\text{Region III}), \quad (6)$$

where m and M are constants, and taking eventually the limit $M \rightarrow \infty$. This guarantees that the confinement process avoids the excitation of negative energy Dirac sea particles, since the plane wave energy spectrum of positive and negative energy solutions is separated by at least twice their mass times c^2 . Thus, the general form of the wavefunction for a bounded Dirac particle in a one dimensional box, vanishing when $|z| \rightarrow \infty$, can be written (in all three regions) as

$$\psi_I = A e^{-iKz} \begin{pmatrix} \chi \\ -R\sigma_z\chi \end{pmatrix} \quad (7)$$

$$\psi_{II} = B e^{ikz} \begin{pmatrix} \chi \\ r\sigma_z\chi \end{pmatrix} + C e^{-ikz} \begin{pmatrix} \chi \\ -r\sigma_z\chi \end{pmatrix} \quad (8)$$

$$\psi_{III} = D e^{iKz} \begin{pmatrix} \chi \\ R\sigma_z\chi \end{pmatrix} \quad (9)$$

where $K = \sqrt{E^2 - (Mc^2)^2}/(\hbar c)$ (an imaginary wavenumber when $M > E/c^2$) and $R = \hbar Kc/(E + Mc^2)$. Thus, in the limit $M \rightarrow \infty$, $K \rightarrow +i\infty$, the terms associated with A and D go to zero. Now, boundary conditions akin to those for the Schrödinger equation, namely $\psi_{II} = 0$ at $z = 0$ and $z = L$ will require ψ_{II} to vanish identically. Thus, they are disallowed. This is related to the fact that the usual boundary conditions for non-relativistic quantum mechanics cannot always be applied to relativistic problems, as was shown by V. Alonso et al. [7]. Instead, we require the outward component of the Dirac current to be zero at the boundaries (the MIT bag model). This ensures that the particle is indeed confined within the box [5].

The conserved current corresponding to Eq.(3) can be shown to be

$$J_z = \bar{\psi}\gamma^z\psi, \quad (10)$$

where $\gamma^z \equiv \gamma^3$ is the z -component of the four-vector set of 4×4 gamma matrices $\gamma^\mu = (\gamma^0, \vec{\gamma})$. These matrices are related to the α_i and β matrices introduced earlier by $\gamma^0 = \beta$ and $\gamma^i = \beta\alpha_i$. The vanishing of the outward component of the Dirac current $J^\mu = \bar{\psi}\gamma^\mu\psi$ at a boundary is obtained by requiring that the condition $i\gamma \cdot n\psi = \psi$ holds there, where n is the unit four-vector normal to the space-time boundary [5], such that $n_\mu n^\mu = -1$. For a static boundary $n^\mu = (0, \hat{x})$, where \hat{x} is the outward normal to the boundary surface. Applying this to the wavefunction ψ_{II} at $z = 0$ and $z = L$ gives [1]

$$i\beta\alpha_z\psi_{II}|_{z=0} = \psi_{II}|_{z=0} \quad (11)$$

$$\text{and } -i\beta\alpha_z\psi_{II}|_{z=L} = \psi_{II}|_{z=L} \quad (12)$$

respectively. Using the expression for ψ_{II} from (8), we get from (11) and (12) respectively

$$\frac{B+C}{B-C} = ir \quad (13)$$

$$\frac{Be^{ikL} + Ce^{-ikL}}{Be^{ikL} - Ce^{-ikL}} = -ir, \quad (14)$$

which in turn yield

$$(ir - 1) = \frac{C}{B}(ir + 1) \quad (15)$$

$$(ir + 1) = \frac{C}{B}(ir - 1)e^{-i2kL}. \quad (16)$$

By eliminating C/B between (15) and (16) one gets

$$\frac{ir - 1}{ir + 1} = e^{ikL} \quad (17)$$

so that we finally arrive to the transcendental equation

$$\tan(kL) = \frac{2r}{r^2 - 1} = -\frac{\hbar k}{mc}. \quad (18)$$

The discrete solutions of this equation for the values of the wavenumber k give the quantized energy levels for a relativistic particle in the 1-dimensional box. Note that the solution with $k = 0$ is excluded because, from (15), $C = -B$ and the upper component would be proportional to $\sin(kx)$ and therefore be identically zero inside the box. It is worth mentioning at this point that Eq. (15) implies that $|B| = |C|$ and this condition could have as well be obtained by just requiring that J_z , given by (10), vanishes at the boundary, as remarked by Menon and Belyi [6]. Note that this condition does not imply that $B = \pm C$, since at least one of B or C is not a real number in this case, as can also be seen from Eq. (15) and the fact that $r \neq 0$. Also one may note that in order to obtain the eigenvalue equation (18), one needs to know the ratio of the complex coefficients C and B , C/B , which we got from the MIT boundary condition, and not only the ratio of their moduli.

To conclude this section, we comment briefly on the negative energy solutions of the Dirac equation (3) in a one-dimensional box. These solutions can be found from the negative energy solutions of the free Dirac equation travelling in opposite directions in the z axis. The new boundary condition is obtained from the corresponding condition for positive energy by applying the charge conjugation operator. The resulting equation for the wavenumber k is identical to (18) and therefore its discrete solutions k_n are the same. This means that one has an overall symmetric energy spectrum, in which for every discrete positive level with energy $E = E_n = \sqrt{\hbar^2 k_n^2 + m^2 c^4}$ there is one with $E = -E_n$. This could be expected, since in our case one has a Dirac Hamiltonian with a confining Lorentz scalar potential which anti-commutes with the charge conjugation operator, as does the free Dirac Hamiltonian. Since the Hamiltonian with the present boundary conditions is Hermitian (see [6]), all wavefunctions belonging to distinct eigenvalues must be orthogonal to each other. Thus the positive and negative energy solutions do not mix. Similar conclusions hold for a two and three dimensional confining box as well.

III. SOLUTION OF DIRAC EQUATION WITH A THREE-DIMENSIONAL INFINITE SQUARE WELL

The generalization of the problem of the previous section involves solving the 3-dimensional Dirac equation with a position-dependent mass of the form

$$m(\vec{r}) = \begin{cases} m & \vec{r} \in V \\ M & \vec{r} \notin V \end{cases}, \quad (19)$$

where V is defined by the set of points with coordinates (x_1, x_2, x_3) such that $0 \leq x_1 \leq L_1$, $0 \leq x_2 \leq L_2$, $0 \leq x_3 \leq L_3$. As before we take the limit $M \rightarrow \infty$. The potential (19) can be written in a more compact way as

$$m(x_1, x_2, x_3) = m + (M - m) \prod_{i=1}^3 [\theta(x_i - L_i) + \theta(-x_i)] \quad (20)$$

where $\theta(x)$ is the step function. For the solutions inside V we expect to have combinations of free Dirac spinors with positive energy, which have the general form

$$\psi = N e^{i\vec{k} \cdot \vec{r}} \begin{pmatrix} \chi \\ r \hat{k} \cdot \vec{\sigma} \chi \end{pmatrix} \quad (21)$$

where \vec{k} is the wave vector and $r = \hbar |\vec{k}| c / (E + mc^2)$.

In the non-relativistic case (i.e., for the Schrödinger equation with free particles confined in the volume V), since the potential (20) is separable, one can use the product ansatz for the wave function

$$\psi = N \prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) \quad (22)$$

and thus turn the three-dimensional problem into a set of three independent one-dimensional problems, the total energy being just the sum of the one-dimensional energies. In the relativistic case, however, one cannot use such an ansatz because of the spinor structure of the wavefunctions. Nevertheless, we may use that feature of the non-relativistic wavefunction as a guide to find the right combination of spinors (21). Indeed, we may require that in the non-relativistic limit, when the lower component of the spinor vanishes, the space part of the remaining 2-component spinor be of the form (22). A wavefunction that meets this requirement is

$$\psi = \begin{pmatrix} \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) \right] \chi \\ \sum_{m=1}^3 \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jm}} e^{-ik_j x_j}) r \hat{k}_m \right] \sigma_m \chi \end{pmatrix} \quad (23)$$

where an overall normalization has been set to unity. It can be easily shown that the above is a superposition, with appropriate products of the coefficients B_i and C_i , of the following 8 eigenfunctions, for all possible combinations of ϵ_i ($i = 1, 2, 3$), with $\epsilon_i = \pm 1$

$$\Psi = e^{i \sum_{i=1}^3 \epsilon_i k_i x_i} \begin{pmatrix} \chi \\ r \sum_{i=1}^3 \epsilon_i \hat{k}_i \sigma_i \chi \end{pmatrix}. \quad (24)$$

Each one of these eigenfunctions is of type (21), and they represent plane waves travelling in the 8 directions $(\pm k_1, \pm k_2, \pm k_3)$ all with the same momentum magnitude $p = \hbar k = \hbar \sqrt{k_1^2 + k_2^2 + k_3^2}$.

Again, we impose the MIT bag boundary conditions $\pm i \beta \alpha_l \psi = \psi$, $l = 1, 2, 3$, with the + and - signs corresponding to $x_l = 0$ and $x_l = L_l$ respectively, ensuring vanishing flux through all six boundaries. First, we write the above boundary condition for any x_l , for the wavefunction given in Eq.(23). This yields the following 2-component equation

$$\begin{aligned} & \pm \begin{pmatrix} i \sum_{m=1}^3 \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jm}} e^{-ik_j x_j}) r \sigma_l \hat{k}_m \sigma_m \right] \chi \\ -i \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) \right] \sigma_l \chi \end{pmatrix} \\ & = \psi. \end{aligned} \quad (25)$$

By equating the upper components of the spinors on each side of this equation and invoke the arbitrariness of χ one gets the matrix relation

$$\begin{aligned} & \prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) I \\ & = \pm i \sum_{m=1}^3 \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jm}} e^{-ik_j x_j}) r \hat{k}_m \sigma_l \sigma_m \right]. \end{aligned} \quad (26)$$

In the same fashion, equating the lower components of the spinors on each side of Eq.(25) and right multiply the

resulting matrix equation by $\pm i \sigma_l$ one gets

$$\begin{aligned} & \pm i \sum_{m=1}^3 \left[\prod_{j=1}^3 \left(B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jm}} e^{-ik_j x_j} \right) r \hat{k}_m \sigma_m \sigma_l \right] \\ &= \prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) I. \end{aligned} \quad (27)$$

Adding these two equations one gets

$$\begin{aligned} & 2 \prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j}) I \\ &= \pm i \sum_{m=1}^3 \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jm}} e^{-ik_j x_j}) r \hat{k}_m \{\sigma_l, \sigma_m\} \right] \\ &= \pm 2i \left[\prod_{j=1}^3 (B_j e^{ik_j x_j} + C_j (-1)^{\delta_{jl}} e^{-ik_j x_j}) r \hat{k}_l \right] I \end{aligned} \quad (28)$$

where the relation $\{\sigma_l, \sigma_m\} = 2\delta_{lm}I$ was used. Noticing that for $j \neq l$ the terms in the products are the same in both sides of the equation, one can divide both sides by $\prod_{j \neq l}^3 (B_j e^{ik_j x_j} + C_j e^{-ik_j x_j})$ and obtain, for each l ,

$$B_l e^{ik_l x_l} + C_l e^{-ik_l x_l} = \pm i (B_l e^{ik_l x_l} - C_l e^{-ik_l x_l}) r \hat{k}_l. \quad (29)$$

Note that the boundary condition (25) gave rise to 3 independent condition pairs, one for each spatial dimension. Eq.(29) yields, at $x_l = 0$ and $x_l = L_l$ respectively

$$B_l + C_l = i (B_l - C_l) r \hat{k}_l \quad (30)$$

and

$$B_l e^{ik_l L_l} + C_l e^{-ik_l L_l} = -i (B_l e^{ik_l L_l} - C_l e^{-ik_l L_l}) r \hat{k}_l. \quad (31)$$

Comparing Eqs.(30) and (31) with Eqs.(13) and (14), we see that we can write, in a similar way as in the previous section,

$$\frac{ir \hat{k}_l - 1}{ir \hat{k}_l + 1} = e^{ik_l L_l} \quad (32)$$

and thus

$$\tan k_l L_l = \frac{2r \hat{k}_l}{r^2 \hat{k}_l^2 - 1} = \frac{2(E + mc^2) \hbar k_l}{\hbar^2 (k_l^2 - k^2) c - 2mc(E + mc^2)}. \quad (33)$$

These are a set of three coupled transcendental equations for k_1, k_2, k_3 that need to be solved to find the energy eigenvalues. Again, the solutions with $k_l = 0$ are excluded. In the non-relativistic limit, $E \sim mc^2$, $\hbar k_l / (mc) = \epsilon_l \ll 1$ so that

$$k_l L_l \sim \arctan(-\epsilon_l) \sim n_l \pi \quad (34)$$

where $n_l = 1, \dots$ so that we recover the well-known quantization conditions for a non-relativistic fermion gas confined in a cubic box.

On the other hand, in the ultra-relativistic limit, when $E \sim \hbar k c \gg mc^2$ and $\hbar k_l / (mc) \gg 1$, one gets

$$k_l L_l \sim \arctan\left(-\alpha \frac{\hbar k_l}{mc}\right) \sim (n_l - 1/2)\pi \quad (35)$$

where α is a coefficient whose value depends on relative magnitude between k_l and the other components (i.e., $\alpha = 1$ if $k_l \gg k_{l'}, l' \neq l$).

The size of the box plays a fundamental role in determining the relativistic behavior of the solutions. Indeed, one may write

$$k_l L_l = \frac{\hbar k_l}{mc} \frac{L_l}{L_C} \quad (36)$$

where $L_C = \hbar/(mc)$ is the Compton wavelength. Given that the righthand side of Eq.(33) is always negative (we take every k_l to be positive) and therefore its first solution such that $\pi/2 < k_l L_l < \pi$, we see that when $L_l \gg L_C$ and $L_l \ll L_C$ we get the non-relativistic and ultra-relativistic limits, respectively. To illustrate this point, we write the eigenvalue equation in terms of ratio L_C/L_l . When k_l is much bigger than the other components, Eq.(33) reads

$$\tan x_l = -x_l \frac{L_C}{L_l} \quad (37)$$

where $x_l = k_l L_l$. The graphical solution of this equation is shown in Fig. 1.

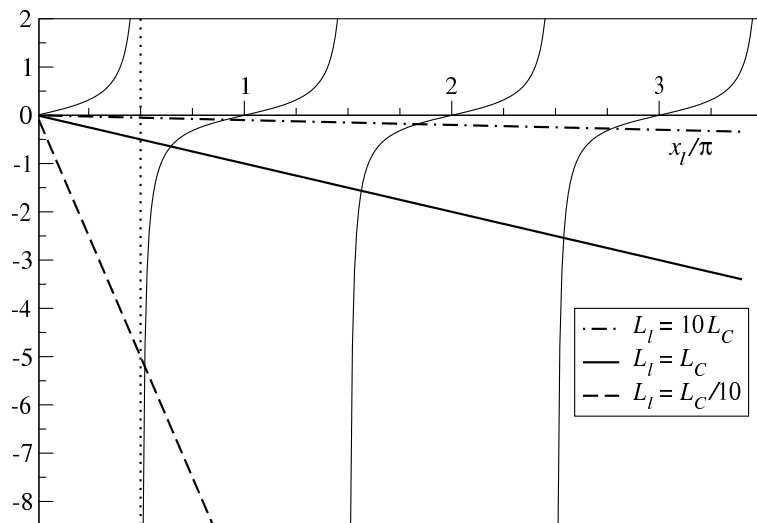


FIG. 1: Graphical solution of equation (37) for three values of the ratio L_l/L_C . The dotted vertical corresponds to $x_l = \pi/2$.

From Fig. 1, one can check that indeed the size of box determines the relativistic nature of the solutions and also that the first non-relativistic solution is $k_l \sim \pi/L_l$ and the first ultra-relativistic solution is $k_l \sim \pi/(2L_l)$. Of course, the degree of relativity increases for the higher energy solutions. Note that if the condition of k_l being much bigger than the other components is relaxed, this would amount to a small change in the coefficient of x_l in the right-end side of Eq.(37), provided that $k_l = \max_i(k_i)$, so that the previous conclusions would still hold. Note that all these conclusions assume that one has always a non-zero mass for the fermions.

In Fig. 2, it is depicted the energy spectra corresponding to the solutions of Eqs. (33) for $L_l = L_C/10$, $L_l = L_C$, $L_l = 10L_C$, considering a cubic box $L_1 = L_2 = L_3$. For convenience, the values plotted are of the logarithm of the scaled kinetic energy $E/(mc^2) - 1$. The levels plotted correspond to the first 27 levels for each value of L_l . However, due to the symmetry of equations (33) with respect to the interchange of the k_l 's among them, some of the levels are degenerate (besides, of course, the spin degeneracy). If $k_1 \neq k_2 \neq k_3$, we have a $3! = 6$ -fold degeneracy, while when $k_l \neq k_{l'} = k_{l''}$, $\{l, l', l''\} = \text{permutations of } \{1, 2, 3\}$, one has a 3-fold degeneracy. This reduces the 27 levels to 10 levels of distinct energies.

This degeneracy is completely analogous to the one found in the non-relativistic case, in which the kinetic energy is given by $E - mc^2 = \hbar^2 \pi^2 / (2mL^2) (n_1^2 + n_2^2 + n_3^2)$, $n_1, n_2, n_3 = 1, \dots, L$ being the size of the cubic box. In fact, one can use the non-relativistic quantum numbers n_l to classify the quantum states in the present case. This is presented in Table I, which contains the quantum numbers, the level degeneracy, the values of $k_l L_l / \pi$ and corresponding energy values for the first 6 distinct energy states.

One can check from the values presented in the table that indeed, for small values of L_l/L_C , k_l approaches $(n_l - 1/2)\pi/L_l$ while for higher values they approach $n_l \pi / L_l$, the non-relativistic value, as suggested by Fig. 1.

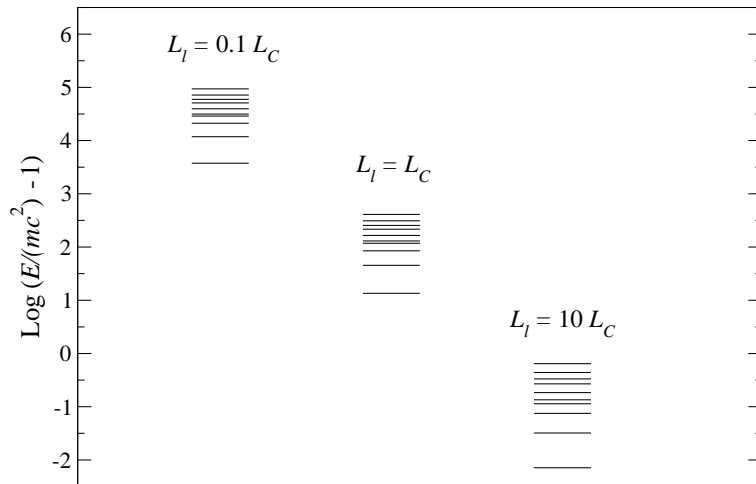


FIG. 2: Scaled kinetic energy spectrum of the first 27 solutions of equation (33) for three values of the ratio L_l/L_C .

| (n_1, n_2, n_3) | degen. | $(k_1, k_2, k_3)(\times L_l/\pi)$ | L_l/L_C | $E/(mc^2)$ |
|-------------------|--------|-----------------------------------|-----------|------------|
| (1,1,1) | 1 | (0.674129, 0.674129, 0.674129) | 0.1 | 36.6957 |
| | | (0.730735, 0.730735, 0.730735) | 1 | 4.10004 |
| | | (0.914156, 0.914156, 0.914156) | 10 | 1.11689 |
| (1,1,2) | 3 | (0.761157, 0.761157, 1.5664) | 0.1 | 59.718 |
| | | (0.789821, 0.789821, 1.61153) | 1 | 6.24063 |
| | | (0.917935, 0.917935, 1.8383) | 10 | 1.22469 |
| (1,2,2) | 3 | (0.800534, 1.62894, 1.62894) | 0.1 | 76.6236 |
| | | (0.820262, 1.66176, 1.66176) | 1 | 7.88349 |
| | | (0.921162, 1.84449, 1.84449) | 10 | 1.32488 |
| (1,1,3) | 3 | (0.819801, 0.819801, 2.53383) | 0.1 | 87.5453 |
| | | (0.835499, 0.835499, 2.56592) | 1 | 8.93086 |
| | | (0.923098, 0.923098, 2.77709) | 10 | 1.38902 |
| (2,2,2) | 1 | (1.66969, 1.66969, 1.66969) | 0.1 | 90.8601 |
| | | (1.69565, 1.69565, 1.69565) | 1 | 9.28075 |
| | | (1.84989, 1.84989, 1.84989) | 10 | 1.41889 |
| (1,2,3) | 6 | (0.838015, 1.69214, 2.57123) | 0.1 | 100.225 |
| | | (0.850724, 1.71438, 2.59869) | 1 | 10.1883 |
| | | (0.92567, 1.85317, 2.7841) | 10 | 1.47937 |

TABLE I: Non-relativistic quantum numbers, degeneracies, values of k_l in units of π/L_l and scaled energies for the first 6 distinct energy solutions of equation (33). For each level are presented the values for $L_l/L_C = 0.1, 1, 10$.

Finally, we will make some considerations regarding density of states of relativistic fermion gases. From Fig. 1 and Table I one sees that as L_l gets bigger each allowed value for k_l is separated by π/L_l as in the non-relativistic fermion gas. For fermion gases confined in large volumes with many particles, as considered for instance in Statistical Physics, the Dirac gas in a 3-D box behaves as a non-relativistic gas. For sizes $V \sim L_C^3$, for which the fermions are relativistic, the density, measured by the separation of k_l values in units of π/L_l , tends to increase, as can be seen from Fig. 1 and Table I, since each solution is separated by less than π/L_l . For smaller volumes, we checked that we recover again the non-relativistic density of states (NRDS) when the quantum numbers changing are relatively high. In general, we can say that, for higher energy levels, the density of states tends to be the same as the NRDS. On the other hand, for small quantum numbers, in relativistic (and ultra-relativistic) conditions, we get higher densities than the NRDS.

IV. CONCLUSIONS

In this paper, we have solved the problem of a relativistic spin-1/2 particle in a three-dimensional square box using the Dirac equation. We studied both the non-relativistic and ultra-relativistic limits and showed that these are related to the size of the box. The scale for gauging the relativity of the solution is the Compton wavelength, such that free fermions confined in boxes with sizes many times the Compton wavelength behave as non-relativistic particles. We solved the three coupled transcendental equations which give the energy eigenvalues of the Dirac particle in a 3D box and used the non-relativistic quantum numbers of quantum particle in a box to classify the corresponding states. We also showed that the density of states is in general higher than the non-relativistic one, but for higher energy states it will tend to be equal to non-relativistic density of states, in which the allowed values for the wavenumber components k_l , $l = 1, 2, 3$ are separated by π/L_l , where L_l is the respective box dimension.

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